Three-fold rotational barrier in CH2=CH-MX3 (M = C, Si, and Ge, and X = F and Cl) and analysis of vibrational spectra of the germanes. Badawi, Hassan M.; Seddigi, Zaki S. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. THEOCHEM (2002), 578 181-189.

Abstract

The structure of CH2:CHMCl3 and CH2:CHMF3 (where M is C, Si, and Ge) series of mols. was studied by DFT-B3LYP/6-311++G** and ab initio MP2/6-311++G** calcns. The sym. potential functions for the internal rotation of the MX3 rotors were calcd. and are in the order: CX3 > SiX3 > GeX3 for the mols. The vibrational frequencies were computed. The decrease in the MX3 rotational barrier is attributed to the decrease in the C-M covalent bond character as going from C to Si to Ge. The potential energy distributions PED among symmetry coordinates of the normal modes of vinyl trihalogermanes were calcd. from normal coordinate calcns.